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Welcome to STN International! Enter x:x

LOGINID: SSPTAJRK1626

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * * * * * * Welcome to STN International * * * * * * * * * * * * * * *

| | | |
|--------------|--|--|
| NEWS 1 | Web Page URLs for STN Seminar Schedule - N. America | |
| NEWS 2 | "Ask CAS" for self-help around the clock | |
| NEWS 3 | SEP 09 | ACD predicted properties enhanced in REGISTRY/ZREGISTRY |
| NEWS 4 | OCT 03 | MATHDI removed from STN |
| NEWS 5 | OCT 04 | CA/CAplus-Canadian Intellectual Property Office (CIPO) added to core patent offices |
| NEWS 6 | OCT 13 | New CAS Information Use Policies Effective October 17, 2005 |
| NEWS 7 | OCT 17 | STN(R) AnaVist(TM), Version 1.01, allows the export/download of CAplus documents for use in third-party analysis and visualization tools |
| NEWS 8 | OCT 27 | Free KWIC format extended in full-text databases |
| NEWS 9 | OCT 27 | DIOGENES content streamlined |
| NEWS 10 | OCT 27 | EPFULL enhanced with additional content |
| NEWS 11 | NOV 14 | CA/CAplus - Expanded coverage of German academic research |
| NEWS 12 | NOV 30 | REGISTRY/ZREGISTRY on STN(R) enhanced with experimental spectral property data |
| NEWS 13 | DEC 05 | CASREACT(R) - Over 10 million reactions available |
| NEWS 14 | DEC 14 | 2006 MeSH terms loaded in MEDLINE/LMEDLINE |
| NEWS 15 | DEC 14 | 2006 MeSH terms loaded for MEDLINE file segment of TOXCENTER |
| NEWS 16 | DEC 14 | CA/CAplus to be enhanced with updated IPC codes |
| NEWS 17 | DEC 16 | MARPATprev will be removed from STN on December 31, 2005 |
| NEWS EXPRESS | DECEMBER 02 CURRENT VERSION FOR WINDOWS IS V8.01,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 02 DECEMBER 2005.
V8.0 USERS CAN OBTAIN THE UPGRADE TO V8.01 AT
http://download.cas.org/express/v8.0-Discover/ | |
| NEWS HOURS | STN Operating Hours Plus Help Desk Availability | |
| NEWS INTER | General Internet Information | |
| NEWS LOGIN | Welcome Banner and News Items | |
| NEWS PHONE | Direct Dial and Telecommunication Network Access to STN | |
| NEWS WWW | CAS World Wide Web Site (general information) | |

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 12:40:55 ON 19 DEC 2005

Page 2

| | | | |
|----------------------|------------|---------|--|
| => file reg | | | |
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL | |
| | ENTRY | SESSION | |
| FULL ESTIMATED COST | 0.21 | 0.21 | |

FILE 'REGISTRY' ENTERED AT 12:41:02 ON 19 DEC 2005
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STRUCTURE FILE UPDATES: 18 DEC 2005 HIGHEST RN 870123-57-2
DICTIONARY FILE UPDATES: 18 DEC 2005 HIGHEST RN 870123-57-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

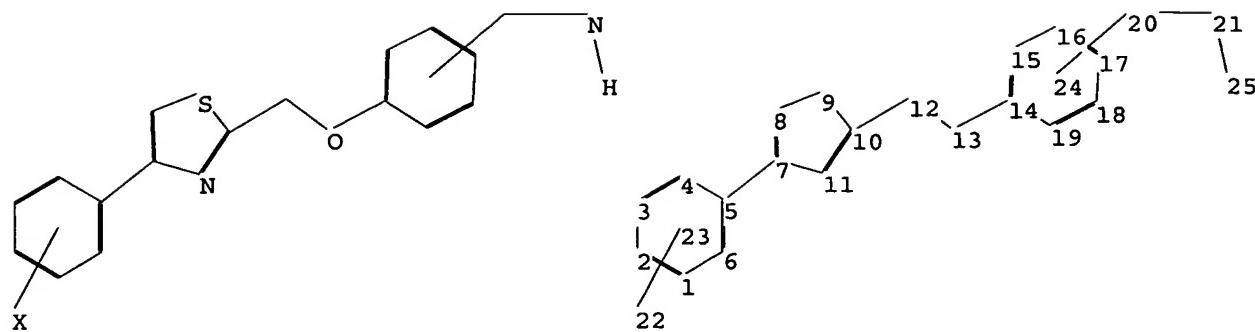
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>
Uploading C:\Program Files\Stnexp\Queries\10612187\Struc 1.str



chain nodes :

12 13 20 21 22 25

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 14 15 16 17 18 19

chain bonds :

5-7 10-12 12-13 13-14 20-21 21-25

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11 14-15 14-19 15-16

16-17 17-18 18-19

exact/norm bonds :

7-8 7-11 8-9 9-10 10-11 12-13 13-14 20-21

exact bonds :

5-7 10-12 21-25

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-19 15-16 16-17 17-18 18-19

Match level :

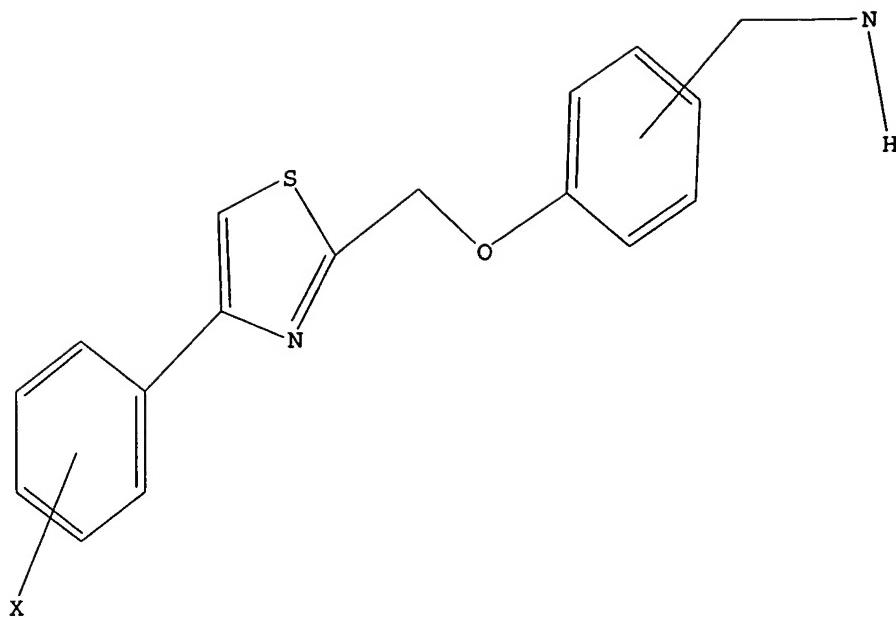
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> l1
SAMPLE SEARCH INITIATED 12:41:17 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 64 TO ITERATE

100.0% PROCESSED 64 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 800 TO 1760
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> l1 full
FULL SEARCH INITIATED 12:41:21 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1305 TO ITERATE

100.0% PROCESSED 1305 ITERATIONS 15 ANSWERS
SEARCH TIME: 00.00.01

L3 15 SEA SSS FUL L1

=> file caplus medline
COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 161.33 161.54

FILE 'CPLUS' ENTERED AT 12:41:27 ON 19 DEC 2005
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FILE 'MEDLINE' ENTERED AT 12:41:27 ON 19 DEC 2005

=> l3
L4 1 L3

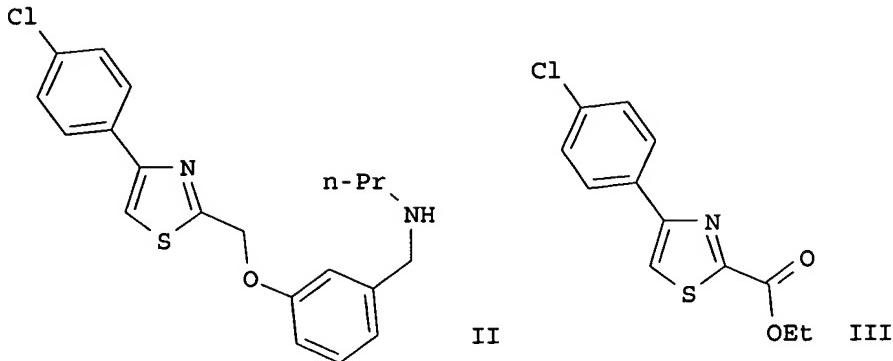
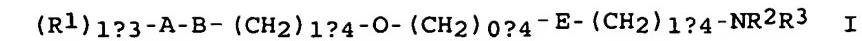
=> d ti

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
TI Preparation of substituted heteroaryl and heterocyclic compounds useful
NAD oxidase hydride donor inhibitors

=> d ibib abs hitstr

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:41452 CAPLUS
DOCUMENT NUMBER: 140:111408
TITLE: Preparation of substituted heteroaryl and heterocyclic
compounds useful NAD oxidase hydride donor inhibitors
INVENTOR(S): Beers, Scott
PATENT ASSIGNEE(S): Janssen Pharmaceutica, N.V., Belg.
SOURCE: PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|--------|------------|-----------------|------------|
| WO 2004005267 | A2 | 20040115 | WO 2003-US20781 | 20030702 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT,
TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 2005014745 | A1 | 20050120 | US 2003-612187 | 20030702 |
| PRIORITY APPLN. INFO.: | | | US 2002-393710P | P 20020703 |
| OTHER SOURCE(S): | MARPAT | 140:111408 | | |
| GI | | | | |



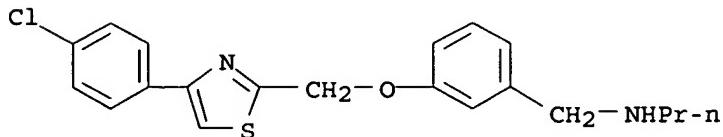
- AB** The invention refers to substituted heteroaryl and heterocyclic compds. I [wherein: R1 is a substituent on the 3, 4 or 5 position of the ring A and R1 = H, alkyl, alkoxy, NH2, NH-alkyl, N(alkyl)2, halogen, OH; A, E = phenylene or pyridinylene; B is a monocyclic 5-membered heteroarylene containing N, O, or S, and optionally containing an addnl. N; R2, R3 = H, alkyl-R4, cycloalkyl; R4 = alkoxy, NH2, NH-alkyl, N(alkyl)2, 1-3 halogen(s), OH, cycloalkyl-R5, heterocyclyl-R5, (hetero)aryl-R5; R5 = H, 1 or 2 of alkyl or alkoxy] and pharmaceutically acceptable salts thereof useful as NAD oxidase hydride donor inhibitors. Compds. I are claimed to be useful in treating or ameliorating reactive oxygen species-mediated inflammatory disorders such as osteoarthritis and Alzheimer's disease. In an NADPH oxidase assay for inhibition of superoxide-mediated reduction of cytochrome c in human neutrophils incubated with phorbol myristate acetate, 11 compds. I had IC50 values of 0.04-3.45 μ M. For instance, compound II (IC50 = 1.65 μ M) was prepared via heterocyclization of 4-ClC6H5C(O)CH2Br with H2NC(S)CO2Et, reduction of obtained thiazole III to the appropriate alc. analog, etherification with 3-HOC6H5CHO, and subsequent reductive amination by propylamine.

IT 646053-15-8P, 3-[[4-(4-Chlorophenyl)-2-thiazolyl]methoxy]-N-propylbenzenemethanamine 646053-17-0P, 4-[[4-(4-Chlorophenyl)-2-thiazolyl]methoxy]-N-propylbenzenemethanamine 646053-18-1P, 3-[[4-(4-Chlorophenyl)-2-thiazolyl]methoxy]-N-(2-methylpropyl)benzenemethanamine 646053-19-2P, 3-[[4-(4-Chlorophenyl)-2-thiazolyl]methoxy]-N-cyclopentylbenzenemethanamine 646053-20-5P, 3-[[4-(4-Chlorophenyl)-2-thiazolyl]methoxy]-N-cyclohexylbenzenemethanamine 646053-21-6P, 3-[[4-(4-Chlorophenyl)-2-thiazolyl]methoxy]-N-cyclopropylbenzenemethanamine 646053-22-7P, N-[3-[[4-(4-Chlorophenyl)-2-thiazolyl]methoxy]phenyl]methyl]-1-methyl-2-pyrrolidinemethanamine dihydrochloride 646053-23-8P, 4-[2-[[3-[[4-(4-Chlorophenyl)-2-thiazolyl]methoxy]phenyl]methyl]amino]ethylmorpholine dihydrochloride 646053-24-9P, 4-(4-Chlorophenyl)-2-[[3-[[[(5-methyl-2-furanyl)methyl]amino]methyl]phenoxy]methyl]thiazole 646053-25-0P, N-[3-[[4-(4-Chlorophenyl)-2-thiazolyl]methoxy]phenyl]methyl]-5-methoxy-1H-indole-3-ethanamine hydrochloride 646053-26-1P, 4-[[4-(4-Chlorophenyl)-2-thiazolyl]methoxy]-N-cyclopentylbenzenemethanamine 646053-27-2P, 3-[[4-(4-Chlorophenyl)-2-thiazolyl]methoxy]benzenemethanamine 646053-30-7P 646053-31-8P 646053-32-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted heteroaryl and heterocyclic compds. as NAD oxidase hydride donor inhibitors useful in treating/ameliorating reactive oxygen species-mediated inflammatory disorders)

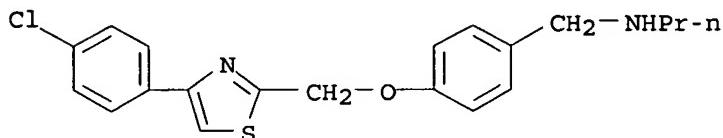
RN 646053-15-8 CAPLUS

CN Benzenemethanamine, 3-[(4-(4-chlorophenyl)-2-thiazolyl)methoxy]-N-propyl- (9CI) (CA INDEX NAME)



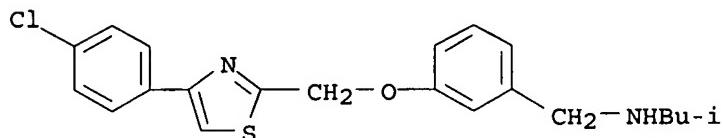
RN 646053-17-0 CAPLUS

CN Benzenemethanamine, 4-[(4-(4-chlorophenyl)-2-thiazolyl)methoxy]-N-propyl- (9CI) (CA INDEX NAME)



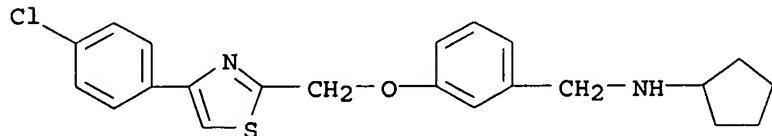
RN 646053-18-1 CAPLUS

CN Benzenemethanamine, 3-[(4-(4-chlorophenyl)-2-thiazolyl)methoxy]-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)



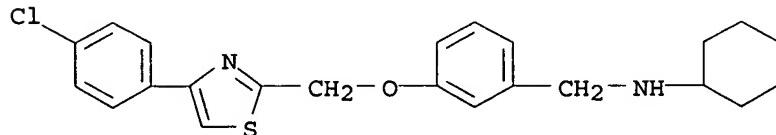
RN 646053-19-2 CAPLUS

CN Benzenemethanamine, 3-[(4-(4-chlorophenyl)-2-thiazolyl)methoxy]-N-cyclopentyl- (9CI) (CA INDEX NAME)



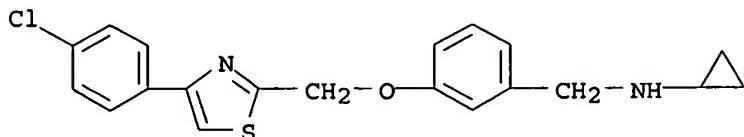
RN 646053-20-5 CAPLUS

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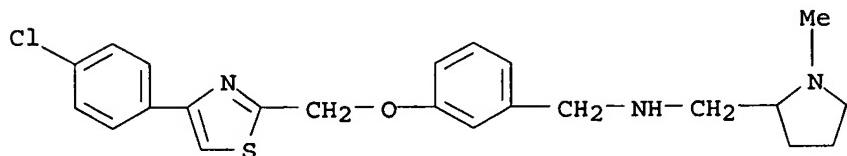
RN 646053-21-6 CAPLUS

CN Benzenemethanamine, 3-[[4-(4-chlorophenyl)-2-thiazolyl]methoxy]-N-cyclopropyl- (9CI) (CA INDEX NAME)



RN 646053-22-7 CAPLUS

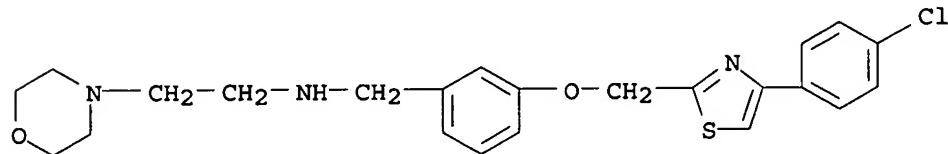
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●2 HCl

RN 646053-23-8 CAPLUS

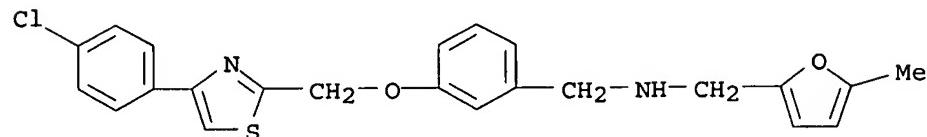
CN 4-Morpholineethanamine, N-[[3-[[4-(4-chlorophenyl)-2-thiazolyl]methoxy]phenyl]methyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 646053-24-9 CAPLUS

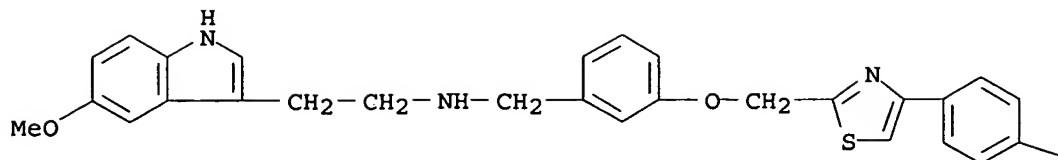
CN 2-Furanmethanamine, N-[[3-[[4-(4-chlorophenyl)-2-thiazolyl]methoxy]phenyl]methyl]-5-methyl- (9CI) (CA INDEX NAME)



RN 646053-25-0 CAPLUS

CN 1H-Indole-3-ethanamine, N-[[3-[[4-(4-chlorophenyl)-2-thiazolyl]methoxy]phenyl]methyl]-5-methoxy-, monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A

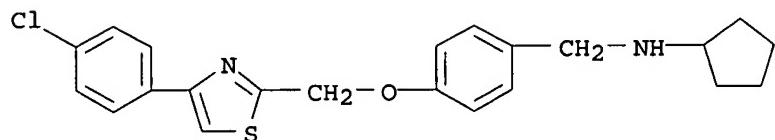


● HCl

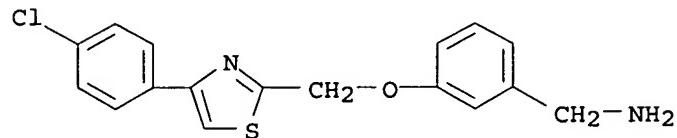
PAGE 1-B

— Cl

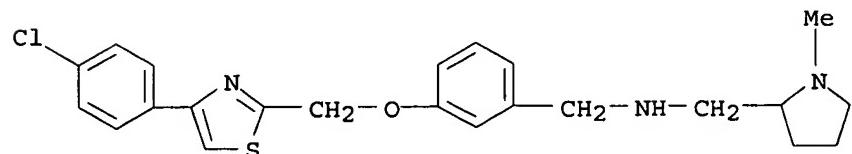
RN 646053-26-1 CAPLUS
CN Benzenemethanamine, 4-[(4-chlorophenyl)-2-thiazolyl]methoxy]-N-cyclopentyl- (9CI) (CA INDEX NAME)



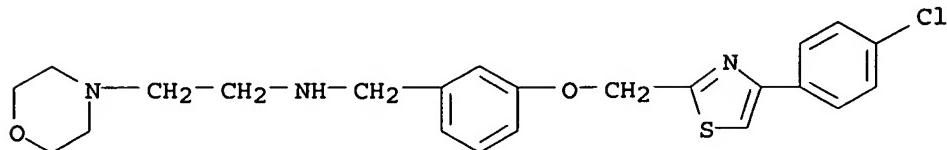
RN 646053-27-2 CAPLUS
CN Benzenemethanamine, 3-[(4-chlorophenyl)-2-thiazolyl]methoxy- (9CI) (CA INDEX NAME)



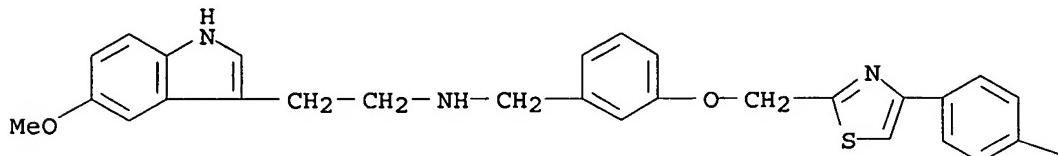
RN 646053-30-7 CAPLUS
CN 2-Pyrrolidinemethanamine, N-[[3-[(4-chlorophenyl)-2-thiazolyl]methoxy]phenyl]methyl- (9CI) (CA INDEX NAME)



RN 646053-31-8 CAPLUS
CN 4-Morpholineethanamine, N-[[3-[[4-(4-chlorophenyl)-2-thiazolyl]methoxy]phenyl]methyl]- (9CI) (CA INDEX NAME)



PAGE 1-A



\ Cl

| | | |
|--|------------|---------|
| => logoff hold | SINCE FILE | TOTAL |
| COST IN U.S. DOLLARS | ENTRY | SESSION |
| FULL ESTIMATED COST | 7.74 | 169.28 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| CA SUBSCRIBER PRICE | ENTRY | SESSION |
| | -0.73 | -0.73 |

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 12:44:48 ON 19 DEC 2005

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAJRK1626

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CAPLUS, MEDLINE' AT 12:56:03 ON 19 DEC 2005
FILE 'CAPLUS' ENTERED AT 12:56:03 ON 19 DEC 2005
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FILE 'MEDLINE' ENTERED AT 12:56:03 ON 19 DEC 2005

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| FULL ESTIMATED COST | 7.74 | 169.28 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | -0.73 | -0.73 |

=> file reg

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| FULL ESTIMATED COST | 7.74 | 169.28 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | -0.73 | -0.73 |

FILE 'REGISTRY' ENTERED AT 12:56:13 ON 19 DEC 2005
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STRUCTURE FILE UPDATES: 18 DEC 2005 HIGHEST RN 870123-57-2
DICTIONARY FILE UPDATES: 18 DEC 2005 HIGHEST RN 870123-57-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

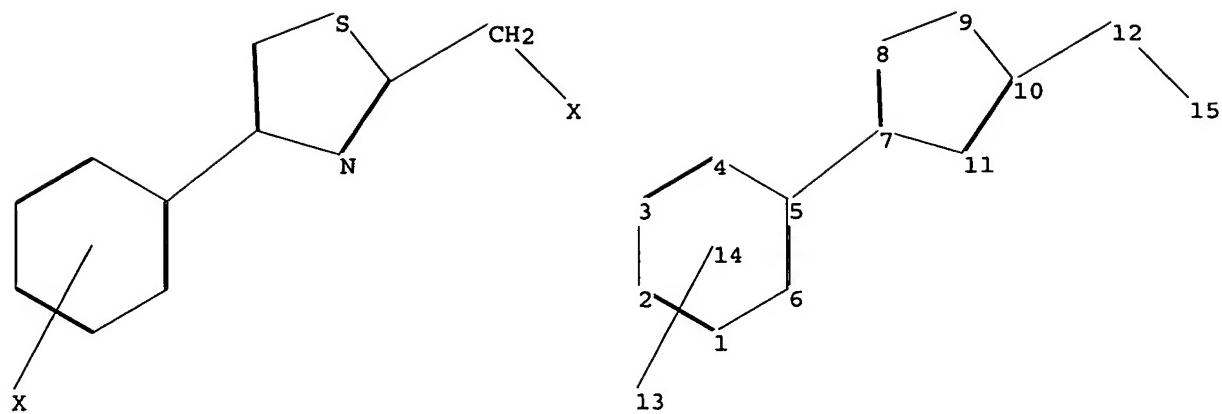
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>
Uploading C:\Program Files\Stnexp\Queries\10612187\Struc 2.str



chain nodes :

12 13 15

ring nodes :

1 2 3 4 5 6 7 8 9 10 11

chain bonds :

5-7 10-12 12-15

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11

exact/norm bonds :

7-8 7-11 8-9 9-10 10-11

exact bonds :

5-7 10-12 12-15

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

Match level :

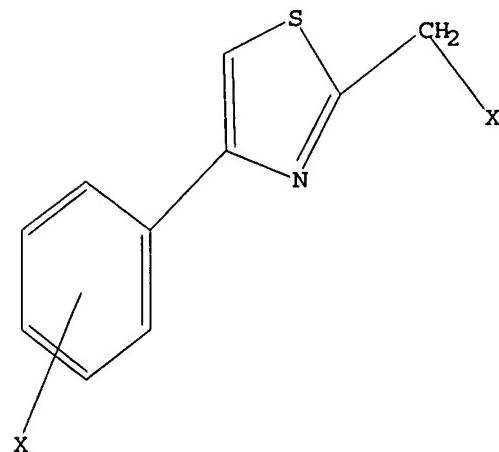
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:CLASS 14:CLASS 15:CLASS

L5 STRUCTURE UPLOADED

=> d

L5 HAS NO ANSWERS

L5 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> 15
SAMPLE SEARCH INITIATED 12:56:28 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 115 TO ITERATE

100.0% PROCESSED      115 ITERATIONS          0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH **COMPLETE**
PROJECTED ITERATIONS:    1657 TO     2943
PROJECTED ANSWERS:        0 TO       0

L6      0 SEA SSS SAM L5

=> 15 full
FULL SEARCH INITIATED 12:56:34 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2461 TO ITERATE

100.0% PROCESSED      2461 ITERATIONS         6 ANSWERS
SEARCH TIME: 00.00.01

L7      6 SEA SSS FUL L5

=> file caplus medline
COST IN U.S. DOLLARS           SINCE FILE      TOTAL
                                ENTRY          SESSION
FULL ESTIMATED COST          161.33          330.61

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE      TOTAL
                                                ENTRY          SESSION
CA SUBSCRIBER PRICE          0.00            -0.73

FILE 'CAPLUS' ENTERED AT 12:56:41 ON 19 DEC 2005
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FILE 'MEDLINE' ENTERED AT 12:56:41 ON 19 DEC 2005

=> 17
L8      5 L7

=> dup rem 18
PROCESSING COMPLETED FOR L8
L9      5 DUP REM L8 (0 DUPLICATES REMOVED)

=> d ibib abs hitstr

L9      ANSWER 1 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:             1995:755717 CAPLUS
DOCUMENT NUMBER:              124:8677
TITLE:                      Evolution of a series of non-quinoline leukotriene D4
                            receptor antagonist; synthesis and SAR of
                            benzothiazoles and thiazoles substituted benzyl
                            alcohols as potent LTD4 antagonists
AUTHOR(S):                  Lau, C. K.; Dufresne, C.; Gareau, Y.; Zamboni, M. ;
                            Labelle, R. N.; Young, K. M.; Metters, C.; Rochette,
                            N.; Sawyer, D. M.; et al.
CORPORATE SOURCE:            Merck Frosst Cent. Therapeutic Res., Pointe
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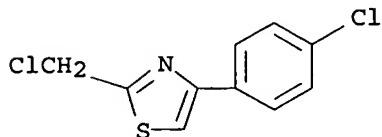
SOURCE: Claire-Dorval, QC, H94 4P8, Can.
 Bioorganic & Medicinal Chemistry Letters (1995),
 5(15), 1615-20
 CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 124:8677

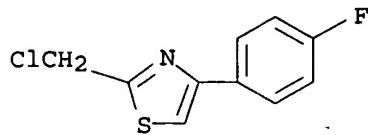
AB Replacement of the quinoline pharmacophore of verlukast by alkylthiazoles and benzothiazoles has lead to the discovery of a new series of potent and orally active LTD4 receptor antagonists. The synthesis and structure activity relationships of this series of compds. are described.

IT 170881-67-1P 170881-68-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and SAR of benzothiazoles and thiazoles substituted benzyl alcs. as potent LTD4 antagonists)

RN 170881-67-1 CAPLUS
 CN Thiazole, 2-(chloromethyl)-4-(4-chlorophenyl)- (9CI) (CA INDEX NAME)



RN 170881-68-2 CAPLUS
 CN Thiazole, 2-(chloromethyl)-4-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



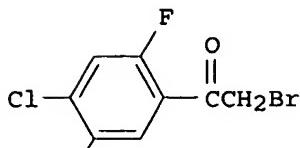
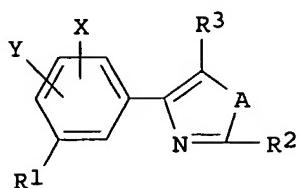
=> d ibib abs hitstr 2-5

L9 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1995:508003 CAPLUS
 DOCUMENT NUMBER: 122:265364
 TITLE: Preparation of 4-phenyloxazole and -thiazole derivatives as herbicides
 INVENTOR(S): Nakanishi, Hiroyuki; Miura, Juzo; Nishioka, Hitoshi; Ootsuka, Takashi
 PATENT ASSIGNEE(S): Nihon Nohyaku Co Ltd, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 47 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|------------|
| JP 06340643 | A2 | 19941213 | JP 1994-89169 | 19940404 |
| PRIORITY APPLN. INFO.: | | | JP 1994-89169 | A 19940404 |
| | | | JP 1993-101921 | 19930404 |

OTHER SOURCE(S) :
GI

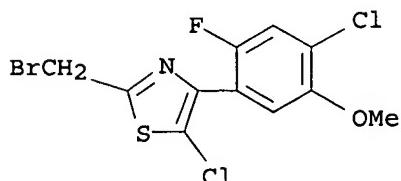
MARPAT 122:265364



AB The title compds. [I; R1 = halo, NO₂, C₁₋₆ alkyl, halosulfonyl, BR4, NR5; wherein B = O, S(O)_n (n = 0-2); R4 = H, C₁₋₆ (halo)alkyl, C₁₋₆ hydroxyalkyl, C₂₋₆ (halo)alkenyl, C₂₋₆ (halo)alkynyl, C₃₋₆ (halo)cycloalkyl, etc.; R5 = H, C₁₋₆ (halo)alkyl, C₂₋₆ (halo)alkenyl, C₂₋₆ (halo)alkynyl, C₃₋₆ cycloalkyl, C₁₋₆ (halo)alkylsulfonyl, phenyl-C₁₋₆ alkyl, etc.; R2 = HO, C₁₋₆ (halo)alkyl, C₁₋₆ cycloalkyl, C₁₋₆ (halo)alkoxy, C₁₋₆ alkoxy-C₁₋₆ alkyl, C₁₋₆ alkylthio-C₁₋₆ alkyl; R3 = H, halo; A = O, S; X, Y = halo, C₁₋₆ (halo)alkyl], which show excellent herbicidal activity against post- and preemergence weeds, are prepared. Thus, 3.10 g 1-bromo-2-phenyl-2-ethanone derivative (II) and 2.61 g isobutyramide were heated at 150-160° for 5.5 h to give, after silica gel chromatog., 81.9% title compound I (R1 = iso-ProO, R2 = iso-Pr, R3 = H; X, Y = 2-F, 4-Cl). I (R1 = OCH₂C.tplbond.CH, R2 = iso-Pr, R3 = Cl; X, Y = 2-F, 4-Cl) at 1 kg/ha postemergence controlled ≥95% Echinochloa crus-galli in a flooded paddy soil and gave no damage to rice. A total of 165 I were prepared.

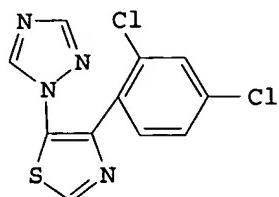
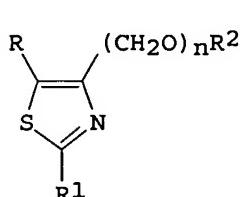
IT 162504-21-4P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of phenyloxazole or -thiazole derivative as herbicide)

RN 162504-21-4 CAPLUS**CN** Thiazole, 2-(bromomethyl)-5-chloro-4-(4-chloro-2-fluoro-5-methoxyphenyl)-(9CI) (CA INDEX NAME)**L9** ANSWER 3 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1991:228903 CAPLUS
 DOCUMENT NUMBER: 114:228903
 TITLE: Preparation of thiazoles as agrochemical fungicides
 INVENTOR(S): Haddock, Ernest; Webb, Suzan Mary
 PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B. V., Neth.
 SOURCE: Eur. Pat. Appl., 31 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------------------------|------|-------------------|-----------------|-------------|
| EP 411718 | A2 | 19910206 | EP 1990-202124 | 19900803 |
| EP 411718 | A3 | 19910703 | | |
| R: CH, DE, FR, GB, IT, LI, NL | | | | |
| JP 03081268 | A2 | 19910405 | JP 1990-205284 | 19900803 |
| US 5332753 | A | 19940726 | US 1992-938687 | 19920901 |
| PRIORITY APPLN. INFO.: | | | GB 1989-17849 | A 19890804 |
| OTHER SOURCE(S): | | MARPAT 114:228903 | US 1990-560567 | B1 19900731 |
| GI | | | | |



AB Thiazoles I [R = H, (CH₂)_mY where m = 0-2 and Y = (substituted) N-containing heterocycle; R₁ = (CH₂)_pX, N(Z)COX, H, (substituted) alkyl, aryl, amino, or aralkyl, p = 0-2, Z = H, alkyl, X = (substituted) N-heterocyclyl; n = 0-2; R₂ = (substituted) Ph] and acid salts, N-oxides, S-oxides and metal salts, were prepared. For example, 2-bromo-2-(1,2,4-triazol-1-yl)-2',4'-dichloroacetophenone (preparation given) was dissolved in EtOH and added to a solution of HC(S)NH₂ in EtOH and the mixture stirred 16 h to give thiazole II in 11% yield. Wheat plants inoculated with Leptosphaeria nodorum at 8 + 105 spores/mL then treated with II at 1 kg/ha showed no fungal growth after 5 days.

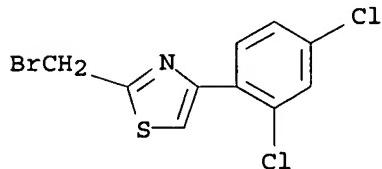
IT 133767-85-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of agrochem. fungicides)

RN 133767-85-8 CAPLUS

CN Thiazole, 2-(bromomethyl)-4-(2,4-dichlorophenyl)- (9CI) (CA INDEX NAME)



L9 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1990:157325 CAPLUS

DOCUMENT NUMBER: 112:157325

TITLE: Dithiocarboxylic acids, dithiocarboxylic esters, or thiocarboxylic amides by reaction of methylene-active chloromethyl compounds with sulfur

AUTHOR(S): Thiel, W.; Mayer, R.

CORPORATE SOURCE: Sekt. Chem., Tech. Univ. Dresden, Dresden, DDR-8027, , Ger. Dem. Rep.

SOURCE: Journal fuer Praktische Chemie (Leipzig) (1989), 331(2), 243-62

CODEN: JPCEAO; ISSN: 0021-8383

DOCUMENT TYPE: Journal
 LANGUAGE: German
 OTHER SOURCE(S): CASREACT 112:157325
 AB With a mixture of S and amine in DMF at room temperature halomethyl compds. can be

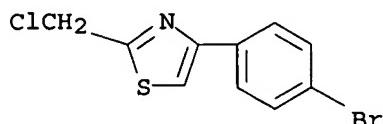
oxidized to give thiocarboxylic acids and their derivs. The reaction was studied in detail especially with chloroacetic derivs. or chloromethyl heterocycles formally derived from chloroacetic acid. The resulting thiooxalic acid derivs. represent activated acids and very useful C2-synthons, especially for the synthesis of heterocycles. Oxidation in the presence of Et₃N leads to dithiocarboxylates which can be alkylated to dithioesters in high yields. As a rule, with different primary and secondary amines instead of tertiary amines these dithiocarboxylates or dithiocarboxylic esters can be transformed already at low temps. to thioamides.

IT 125983-35-9

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with sulfur in presence of amine)

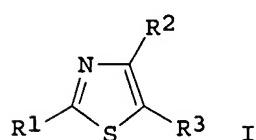
RN 125983-35-9 CAPLUS

CN Thiazole, 4-(4-bromophenyl)-2-(chloromethyl)- (9CI) (CA INDEX NAME)



L9 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1988:112450 CAPLUS
 DOCUMENT NUMBER: 108:112450
 TITLE: Preparation of imidazolylmethylthiazoles as medical fungicides and bactericides
 INVENTOR(S): Takano, Shuntaro; Imaizumi, Hiroyuki; Kajita, Tetsuya; Takashima, Kenichi; Takezawa, Katsushi; Yotsutsuji, Minako; Yasuda, Takashi; Yotsutsuji, Akira; Sakai, Hiroshi; Saikawa, Isamu
 PATENT ASSIGNEE(S): Toyama Chemical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 31 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|----------|
| ----- | ---- | ----- | ----- | ----- |
| JP 62178590 | A2 | 19870805 | JP 1986-16868 | 19860130 |
| JP 07025754 | B4 | 19950322 | | |
| PRIORITY APPLN. INFO.: | | | JP 1986-16868 | 19860130 |
| GI | | | | |



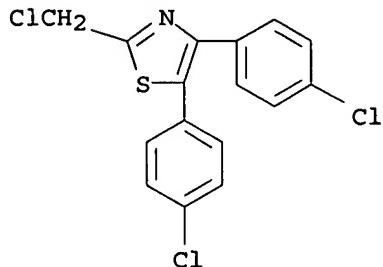
AB The title compds. I [R1-R3 = H, halo, CHO, CO₂H (or esters), (un)substituted alkyl, alkenyl, alkynyl, aryl, cycloalkyl, (CH₂)_nR₄ (R₄ = imidazolyl, 1,2,4-triazolyl, n = 0 or 1); one of R1-R3 is (CH₂)_nR₄], useful as medical fungicides and bactericides, were prepared. A mixture of 630 mg 4-bromomethyl-5-butyl-2-(4-chlorophenyl)thiazole (preparation given) and 595 mg imidazole in 13 mL CHCl₃ was refluxed for 1 h to give 78.7% thiazole derivative I [R₁ = 4-ClC₆H₄, R₂ = (1H-imidazol-1-yl)methyl, R₃ = Bu] (II). II in vitro exhibited a MIC of 6.25 µg/mL against Candida albicans IFO 0583.

IT 113265-00-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate in preparation of medical fungicide and bactericide)

RN 113265-00-2 CAPLUS

CN Thiazole, 2-(chloromethyl)-4,5-bis(4-chlorophenyl)- (9CI) (CA INDEX NAME)



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|--|------------|---------|--|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL | |
| | ENTRY | SESSION | |
| FULL ESTIMATED COST | 26.10 | 356.71 | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL | |
| | ENTRY | SESSION | |
| CA SUBSCRIBER PRICE | -3.65 | -4.38 | |

STN INTERNATIONAL LOGOFF AT 12:58:19 ON 19 DEC 2005